

Software and HSF Report October 2020 – March 2021

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Simulation

The new release of Geant4 10.7 has been deployed on schedule last December. A first Beta version of a new optional tasking system is provided with the new release; it is based on the [Parallel Tasking Library \(PTL\)](#), configured as such it can optionally replace the traditional POSIX threads implementation by enabling at run-time the use of tasks for controlling the event loop. The implementation is fully compatible with Intel/TBB, which can be selected as alternative and enabled at configuration time.

The code has been optimized in different areas, particularly in the handling of internal data structures, in the transportation algorithms and through the adoption of C++11 features; all contributing to roughly 5-7% CPU speedup measured on most observables, compared to the previous release series.

The build configuration system has been extended in view of future support of modular libraries builds; the built-in Python module, G4Py, can be now enabled directly at configuration. The new release also includes a better integration and new settings for the [TiMemory](#) built-in profiling tool and comes with a new performance regression testing suite. New templated classes for equation of motion and selected field steppers are now available, together with more accurate diagnostics for propagation in field. New scoring features are also introduced and together with a new UI messenger for hadronic processes, to control the level of verbosity from hadronic physics.

A new electro-magnetic model for polarized gamma elastic scattering is included, as well as a new Coulomb scattering model for e^+/e^- based on very accurate Differential Cross-Sections using *Dirac Partial Wave Analysis*. The new release also comes with a new thermal model of positronium decay to gammas and a new model for gamma-ray elastic interactions, able to account for molecular interference effects. The Glauber-Gribov approach has been extended to cover heavy hadrons, for charm and bottom hadron-nuclear (elastic and inelastic) cross-sections. The treatment of anti-baryon interactions in the Quark-Gluon-String (QGS) model has been improved and a new coalescence model, useful in particular for Cosmic Ray applications has been introduced. Also included a new utility to access hadronic processes, allowing to customise hadronic cross-sections per particle type.

The new release 10.7 comes paired to a new version 1.1.9 of the VecGeom library, which includes several improvements to the build system, new navigation options supporting its use on GPU devices and bug-fixes.

There are detailed [release notes](#) for release 10.7. A first patch release of Geant4, 10.7.p01 has been also released in February. The patch includes [fixes in several areas](#), addressing also issues reported by LHC experiments.

The Geant4 validation portal (geant-val.cern.ch) has been further improved; it has migrated to adopt the latest Angular version; new enhanced UI is now available, and a more friendly representation/display of results is now possible; included are also new features, like static/JavaScript ROOT plots and new LaTeX formula renderer.

The Geant4 web site has migrated to Drupal-8.

Following the successful courses held last year, a new course for beginners on Geant4 is being organized for end of May as part of the official CERN Technical Training program. An advanced course is also being planned for later in fall.

The 2021 workplan of Geant4 was presented and discussed in the last [Technical Forum](#) as well as in [SFT Meetings](#). The next collaboration meeting will be September 20-24th.

ROOT

ROOT is about to release the new production version v6.24. It comes with an updated LLVM to provide support for C++17, the result of work that started a year ago. ROOT 6.24 includes several new features, improvements and bug fixes. Most notable are support for Bearer Tokens and a preview of distRDF (distributed RDataFrame) for distributed analysis, a feature developed over the last two years. It is based on the very successful RDataFrame analysis interface and is designated to supersede PROOF. Worth mentioning are also an architecture-independent, yet high-performance, version of RanLux++; the automatic use of architecture-specific accelerated RooFit libraries; and a major upgrade of JSROOT, ROOT's JavaScript interface used by several external tools and ROOT's WebGUI.

The R&D efforts are seeing significant progress, for instance with benchmarks of RNTuple on HPC and of a DAOS-based object-store backend for RNTuple. ROOT has published its plan of work for 2021, which is the result of the team's consultations with experiments.

The ROOT Plan of Work for 2021 was presented and discussed with the experiments and in SFT Meetings ([1](#), [2](#)).

CernVM-FS

During fall 2020 and spring 2021, the CernVM-FS 2.7.5 patch version and the CernVM-FS 2.8 feature version were released. The releases close some 20 bug reports and provide new support for “template transactions” (fast publishing of meta-data only changes), an ephemeral writable shell for greater flexibility of publishing workflows as well as the integration with the containerd and podman industry products that can now use container images hosted in cvmfs. Platform support was extended to Windows via the Windows Subsystem for Linux (WSL-2), macOS 11 (Intel and M1 architectures), and kubernetes.

On the infrastructure side, all CernVM-FS repositories at CERN were migrated to the central Ceph/S3 storage service in collaboration with IT-ST. The CernVM-FS gateway services were improved to enable multiple concurrent publishers for the LHCb nightly build services, allowing LHCb for the first time to publish the full set of nightly builds on CernVM-FS. The CernVM-FS website cernvm.cern.ch migrated from Drupal to Jekyll. A new monitoring site for repository maintainers was deployed. A new CernVM discourse forum for support and discussion was set up, aiming at replacing the support mailing lists.

The CernVM-FS team participated in training efforts through an EGI webinar (~50 participants from 16 countries) and an “EGI clinic” on CernVM-FS. On 1-2 February, the CernVM Workshop took place with 99 registered participants. New features and use cases from experiments, HPC environments, and container workflows were presented.

The current developments, summarised in the [plan of work](#), are focused on connecting the CernVM-FS container publishing service directly to the central CERN container registries and on the consolidation of the new features. CernVM-FS 2.9 is expected in H2/2020.

CernVM

In January, CernVM 4.5 was released as a minor release following EL 7.9 upstream changes. The NA48 collaboration has become a new user of the CernVM services for long-term software preservation.

Software Process and Infrastructure

This period was mostly devoted to the consolidation of the layer technology, with the preparation of several layers for LHCb (based on LCG_97a) and ATLAS (based on LCG_98). There was streamlining of the build infrastructure, with the introduction of Jenkins pipelines both for nightlies and releases, and to a significant improvement in the reutilisation of binary artifacts through better caching.

The period also saw the transition to Python version 3 as the default and the validation of the new PyROOT module, which was finally available in ROOT v6.22/04.

To mark the changes introduced by these achievements, the SPI team decided to go for a new major release, LCG_99, based on ROOT v6.22/06 and Python 3.8.6, which was announced on 18 January 2021.

On the development side, beside the usual consolidation work, especially for incremental builds, investigations of the container-based CernVM-FS publication has started, based on the features introduced in the recent CernVM-FS 2.8. The execution of the Gaudi tests was included in the nightly builds to speed up the discovery of issues for this central package. Investigation of the Spack package manager continued, and the available set of packages integrated with many updates of recipes, in particular for ROOT; part of this work has been done together with the Turnkey Software Stack (Key4hep) developers. The full plan of work was [discussed in January](#).

HEP Software Foundation Activities and News

As a follow-up to the successful May virtual workshop the HSF and WLCG organised a [second November workshop](#), on the HSF side this time more focussed on specific software matters: working group updates, detector simulation, event generators and a very popular open call R&D session (the first time we did this, to which the community submitted twice the number of talks than we could accommodate in the end). Post-workshop survey feedback was very positive.

We have been strengthening links with the nuclear physics community and the HSF has joined JLab and BNL in organising the [Software and Computing Roundtable](#) meeting series with HSF speakers and common topics with nuclear physics.

Together with colleagues working towards the Software Institute for Data Intensive Science (SIDIS) and openlab a new series of meetings has started, the [Compute Accelerator Forum](#), which mixes technical presentations from industry with HEP-specific software presentations on the use of accelerators. Monthly meetings are now well established and proving popular (~70 participants).

Training activities have been extremely popular, with two editions of a HEP C++ course being run that has been up to x5 over-subscribed (all places for the last edition were grabbed in under 3 minutes!). CI/CD training was also run in 2021, reaching close to 200 students. Development of new training material is being helped by events such as the [Software Training Hackathon](#) in December. All this training is resourced by volunteers and providing more recognition and support for this work is needed.

The HSF also engaged this year in a [planning exercise](#), helping to engage the community more in the activities of the working groups. Some new activities, such as the PyHEP WG “Module of the Month” series, are already attracting a lot of interest.

Finally, preparations for the second phase of the HL-LHC Computing Review have begun, with many HSF members involved, together with the LHC experiments and WLCG.